



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:01 AM UTC

PDB ID : 9CA6 / pdb_00009ca6
Title : Rns Pocket Mutant - I14F/I17F
Authors : Tolbert, J.D.; Midgett, C.R.; Kull, F.J.
Deposited on : 2024-06-17
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

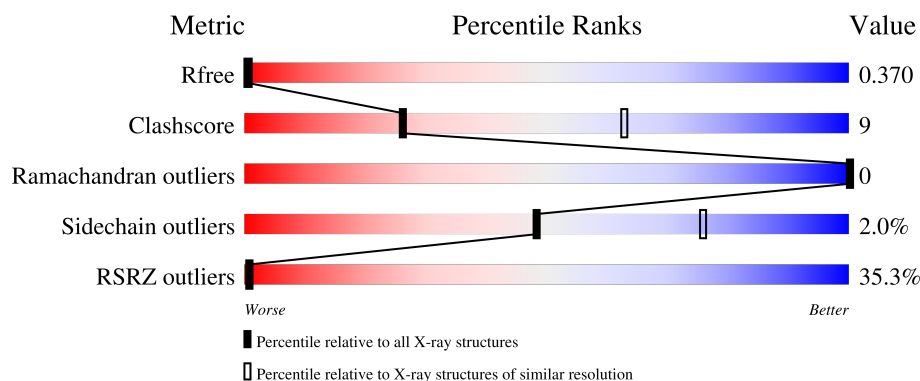
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	265	32% 67% 22% 9%
1	B	265	32% 66% 22% 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3941 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Regulatory protein Rns.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1967	1264	330	361	12			
1	B	241	Total	C	N	O	S	0	0	0
			1974	1267	331	364	12			

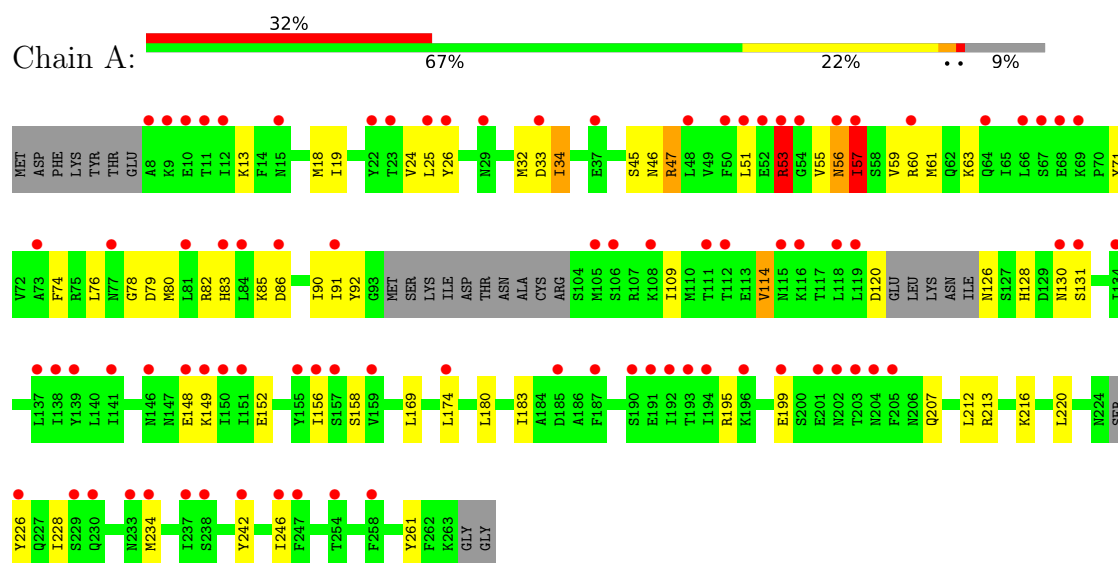
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ALA	GLU	conflict	UNP P16114
A	14	PHE	ILE	engineered mutation	UNP P16114
A	17	PHE	ILE	engineered mutation	UNP P16114
B	8	ALA	GLU	conflict	UNP P16114
B	14	PHE	ILE	engineered mutation	UNP P16114
B	17	PHE	ILE	engineered mutation	UNP P16114

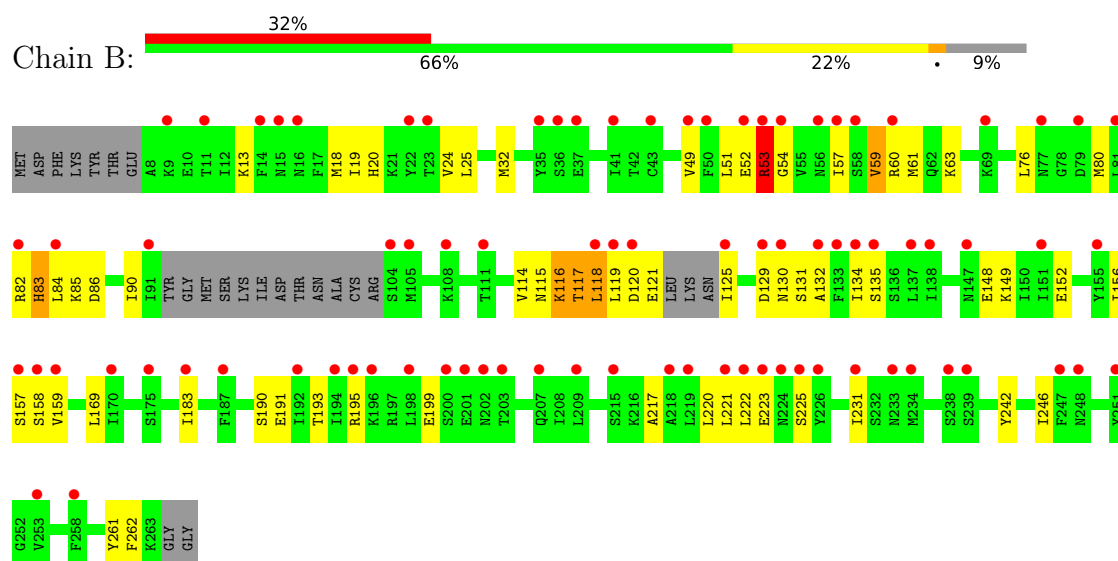
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Regulatory protein Rns



• Molecule 1: Regulatory protein Rns



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.81Å 96.68Å 138.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.20 – 3.00 29.20 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.20-3.00) 83.2 (29.20-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.58 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.352 , 0.369 0.353 , 0.370	Depositor DCC
R_{free} test set	1336 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.9	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	3941	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6057e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	10/1997 (0.5%)	0.84	19/2677 (0.7%)
1	B	0.67	3/2004 (0.1%)	0.74	10/2688 (0.4%)
All	All	0.72	13/4001 (0.3%)	0.79	29/5365 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	SER	C-N	-18.88	1.07	1.33
1	B	83	HIS	C-N	-17.64	1.11	1.33
1	B	59	VAL	C-N	-13.37	1.14	1.33
1	A	57	ILE	C-N	-11.36	1.18	1.33
1	B	82	ARG	C-N	10.93	1.47	1.33
1	A	79	ASP	C-N	9.30	1.46	1.33
1	A	83	HIS	C-N	-8.56	1.22	1.33
1	A	82	ARG	C-N	7.15	1.43	1.33
1	A	47	ARG	C-N	7.04	1.43	1.33
1	A	78	GLY	C-N	7.00	1.43	1.33
1	A	56	ASN	C-N	6.46	1.41	1.33
1	A	91	ILE	C-N	6.38	1.43	1.33
1	A	126	ASN	C-N	-6.15	1.26	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	SER	O-C-N	-12.32	107.62	122.65
1	A	34	ILE	O-C-N	-10.45	111.44	123.03
1	B	59	VAL	O-C-N	9.73	133.57	123.07
1	B	82	ARG	CA-C-N	-9.64	107.91	120.44
1	B	82	ARG	C-N-CA	-9.64	107.91	120.44
1	B	83	HIS	O-C-N	-9.53	112.26	122.07
1	A	79	ASP	O-C-N	9.27	132.10	122.09
1	A	45	SER	CA-C-N	8.36	137.51	121.54
1	A	45	SER	C-N-CA	8.36	137.51	121.54
1	A	78	GLY	CA-C-N	-8.11	109.41	120.44
1	A	78	GLY	C-N-CA	-8.11	109.41	120.44
1	A	47	ARG	O-C-N	-7.54	113.96	123.24
1	B	117	THR	N-CA-C	-7.54	103.81	113.16
1	A	57	ILE	O-C-N	-7.24	114.93	122.82
1	A	47	ARG	CA-C-N	7.01	132.46	122.09
1	A	47	ARG	C-N-CA	7.01	132.46	122.09
1	B	59	VAL	CA-C-N	-6.67	113.33	123.07
1	B	59	VAL	C-N-CA	-6.67	113.33	123.07
1	A	78	GLY	O-C-N	6.50	128.89	122.19
1	A	33	ASP	CA-C-N	-6.04	115.32	122.93
1	A	33	ASP	C-N-CA	-6.04	115.32	122.93
1	A	83	HIS	O-C-N	-5.79	115.98	122.12
1	B	118	LEU	N-CA-C	-5.39	105.30	111.07
1	A	82	ARG	O-C-N	-5.33	116.58	122.07
1	A	34	ILE	CA-C-N	5.21	130.19	123.00
1	A	34	ILE	C-N-CA	5.21	130.19	123.00
1	B	116	LYS	N-CA-C	5.15	115.81	108.54
1	A	128	HIS	N-CA-C	-5.07	108.12	114.56
1	B	223	GLU	N-CA-C	-5.05	107.16	113.72

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	ARG	Sidechain
1	A	53	ARG	Sidechain
1	A	57	ILE	Mainchain
1	B	53	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1967	0	2011	38	1
1	B	1974	0	2022	41	1
All	All	3941	0	4033	75	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (75) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:VAL:HG11	1:B:117:THR:CG2	1.94	0.95
1:B:114:VAL:HG11	1:B:117:THR:HG23	1.53	0.91
1:B:114:VAL:CG1	1:B:117:THR:HG23	2.07	0.84
1:A:34:ILE:HG23	1:A:57:ILE:HD12	1.69	0.75
1:B:114:VAL:HG11	1:B:117:THR:HG22	1.72	0.71
1:A:46:ASN:O	1:A:114:VAL:HG22	1.93	0.69
1:A:55:VAL:HG12	1:A:57:ILE:HG23	1.73	0.68
1:B:217:ALA:O	1:B:221:LEU:HG	1.94	0.68
1:A:90:ILE:HD13	1:B:86:ASP:HB3	1.77	0.66
1:A:13:LYS:HD3	1:A:60:ARG:HB2	1.78	0.66
1:A:55:VAL:HG12	1:A:57:ILE:CG2	2.25	0.65
1:A:130:ASN:OD1	1:A:131:SER:N	2.29	0.64
1:B:32:MET:HE2	1:B:61:MET:HE3	1.80	0.63
1:B:222:LEU:HD22	1:B:262:PHE:HB2	1.79	0.63
1:B:13:LYS:HD3	1:B:60:ARG:HB2	1.81	0.62
1:B:115:ASN:OD1	1:B:116:LYS:N	2.33	0.62
1:A:32:MET:HE2	1:A:61:MET:HE3	1.80	0.61
1:A:34:ILE:CG2	1:A:57:ILE:HD12	2.31	0.60
1:A:85:LYS:HD3	1:A:158:SER:OG	2.04	0.58
1:B:220:LEU:CD1	1:B:231:ILE:HG23	2.34	0.57
1:B:85:LYS:HD3	1:B:158:SER:OG	2.04	0.57
1:A:152:GLU:O	1:A:156:ILE:HG12	2.06	0.56
1:B:59:VAL:HG12	1:B:61:MET:HG2	1.89	0.55
1:B:19:ILE:O	1:B:53:ARG:HA	2.08	0.54
1:B:114:VAL:HG12	1:B:117:THR:HG23	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:LEU:HD12	1:B:231:ILE:HG23	1.90	0.53
1:B:129:ASP:OD1	1:B:131:SER:N	2.42	0.52
1:A:169:LEU:HD23	1:A:183:ILE:HG13	1.92	0.51
1:A:226:TYR:CE2	1:A:234:MET:HB2	2.46	0.51
1:B:148:GLU:HG2	1:B:149:LYS:N	2.25	0.51
1:A:63:LYS:HG3	1:A:261:TYR:CZ	2.47	0.50
1:B:63:LYS:HG3	1:B:261:TYR:CZ	2.46	0.50
1:B:52:GLU:HG2	1:B:157:SER:HB3	1.93	0.49
1:B:53:ARG:NH2	1:B:159:VAL:O	2.45	0.49
1:A:19:ILE:O	1:A:53:ARG:HA	2.13	0.49
1:B:119:LEU:O	1:B:121:GLU:HG3	2.13	0.49
1:A:90:ILE:HD12	1:B:90:ILE:HD12	1.95	0.48
1:B:83:HIS:O	1:B:84:LEU:C	2.52	0.48
1:A:220:LEU:HD22	1:A:226:TYR:HD1	1.79	0.48
1:B:152:GLU:O	1:B:156:ILE:HG12	2.13	0.48
1:A:74:PHE:CZ	1:A:120:ASP:OD2	2.67	0.47
1:A:55:VAL:CG1	1:A:57:ILE:CG2	2.91	0.47
1:B:169:LEU:HD23	1:B:183:ILE:HG13	1.96	0.47
1:A:212:LEU:O	1:A:216:LYS:HG2	2.14	0.47
1:A:18:MET:HB2	1:A:56:ASN:HD22	1.80	0.46
1:B:190:SER:O	1:B:193:THR:OG1	2.32	0.46
1:A:220:LEU:HD22	1:A:226:TYR:CD1	2.50	0.46
1:B:20:HIS:O	1:B:53:ARG:HG3	2.15	0.46
1:B:195:ARG:O	1:B:199:GLU:HG2	2.16	0.46
1:B:242:TYR:O	1:B:246:ILE:HG12	2.17	0.45
1:A:195:ARG:O	1:A:199:GLU:HG2	2.16	0.44
1:B:18:MET:CE	1:B:54:GLY:HA2	2.48	0.44
1:B:130:ASN:O	1:B:134:ILE:HG12	2.18	0.43
1:A:74:PHE:CE1	1:A:120:ASP:OD2	2.72	0.43
1:B:132:ALA:O	1:B:135:SER:OG	2.30	0.43
1:B:25:LEU:O	1:B:49:VAL:N	2.51	0.42
1:A:86:ASP:HB3	1:B:90:ILE:HD13	2.00	0.42
1:B:76:LEU:HA	1:B:80:MET:HE3	2.00	0.42
1:A:242:TYR:O	1:A:246:ILE:HG12	2.19	0.42
1:A:55:VAL:HG12	1:A:57:ILE:HG21	2.02	0.42
1:A:180:LEU:HD21	1:A:195:ARG:HG3	2.02	0.42
1:B:148:GLU:HG2	1:B:149:LYS:HG3	2.01	0.42
1:A:92:TYR:CD2	1:B:131:SER:HB2	2.55	0.41
1:B:121:GLU:HB2	1:B:125:ILE:HA	2.02	0.41
1:A:55:VAL:HG11	1:A:109:ILE:HD11	2.02	0.41
1:A:61:MET:HB3	1:A:61:MET:HE2	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLU:HG2	1:A:149:LYS:N	2.35	0.41
1:A:174:LEU:HD12	1:A:174:LEU:HA	1.97	0.41
1:A:25:LEU:HD13	1:A:51:LEU:HD11	2.02	0.41
1:B:120:ASP:O	1:B:121:GLU:C	2.63	0.41
1:A:76:LEU:HA	1:A:80:MET:HE3	2.02	0.41
1:B:191:GLU:O	1:B:195:ARG:HG3	2.21	0.41
1:A:26:TYR:O	1:A:71:TYR:HB2	2.21	0.41
1:A:174:LEU:O	1:A:213:ARG:NH2	2.53	0.41
1:A:59:VAL:HG12	1:A:61:MET:HG2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLN:NE2	1:B:225:SER:O[2_455]	1.97	0.23

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	232/265 (88%)	225 (97%)	7 (3%)	0	100	100
1	B	235/265 (89%)	227 (97%)	8 (3%)	0	100	100
All	All	467/530 (88%)	452 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	224/246 (91%)	220 (98%)	4 (2%)	51	77
1	B	226/246 (92%)	221 (98%)	5 (2%)	45	74
All	All	450/492 (92%)	441 (98%)	9 (2%)	48	76

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	53	ARG
1	A	114	VAL
1	A	228	ILE
1	B	24	VAL
1	B	51	LEU
1	B	53	ARG
1	B	57	ILE
1	B	118	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	248	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	57:ILE	C	58:SER	N	1.18
1	B	59:VAL	C	60:ARG	N	1.14
1	B	83:HIS	C	84:LEU	N	1.11
1	A	45:SER	C	46:ASN	N	1.07

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	240/265 (90%)	1.84	86 (35%)  	60, 78, 98, 107	0
1	B	241/265 (90%)	1.76	84 (34%)  	60, 76, 91, 112	0
All	All	481/530 (90%)	1.80	170 (35%)  	60, 77, 96, 112	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	202	ASN	6.9
1	B	159	VAL	5.5
1	B	201	GLU	5.5
1	A	203	THR	5.3
1	A	156	ILE	5.0
1	B	130	ASN	5.0
1	A	23	THR	4.9
1	A	11	THR	4.8
1	B	157	SER	4.5
1	B	234	MET	4.3
1	A	67	SER	4.3
1	B	222	LEU	4.2
1	A	194	ILE	4.2
1	A	112	THR	4.1
1	A	201	GLU	4.1
1	B	233	ASN	4.0
1	A	50	PHE	4.0
1	A	226	TYR	3.9
1	A	229	SER	3.8
1	B	221	LEU	3.8
1	A	155	TYR	3.8
1	B	187	PHE	3.8
1	A	187	PHE	3.8
1	A	202	ASN	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	196	LYS	3.8
1	A	205	PHE	3.8
1	A	51	LEU	3.7
1	A	151	ILE	3.6
1	A	77	ASN	3.6
1	A	234	MET	3.6
1	A	157	SER	3.6
1	B	105	MET	3.5
1	A	68	GLU	3.5
1	B	194	ILE	3.4
1	B	225	SER	3.3
1	A	192	ILE	3.3
1	B	155	TYR	3.3
1	A	12	ILE	3.2
1	B	248	ASN	3.2
1	A	190	SER	3.2
1	B	58	SER	3.1
1	B	247	PHE	3.1
1	A	115	ASN	3.1
1	A	53	ARG	3.1
1	B	50	PHE	3.0
1	B	223	GLU	3.0
1	A	105	MET	3.0
1	B	84	LEU	3.0
1	B	36	SER	3.0
1	B	133	PHE	3.0
1	B	258	PHE	3.0
1	A	84	LEU	2.9
1	A	238	SER	2.9
1	B	52	GLU	2.9
1	B	54	GLY	2.9
1	B	239	SER	2.9
1	B	198	LEU	2.9
1	B	111	THR	2.9
1	A	106	SER	2.8
1	A	159	VAL	2.8
1	A	146	ASN	2.8
1	A	81	LEU	2.8
1	A	199	GLU	2.8
1	B	138	ILE	2.8
1	A	204	ASN	2.8
1	B	119	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	57	ILE	2.8
1	B	224	ASN	2.7
1	A	26	TYR	2.7
1	A	233	ASN	2.7
1	B	134	ILE	2.7
1	B	104	SER	2.7
1	A	73	ALA	2.7
1	A	174	LEU	2.7
1	B	207	GLN	2.7
1	B	81	LEU	2.7
1	A	86	ASP	2.7
1	A	10	GLU	2.6
1	A	254	THR	2.6
1	B	43	CYS	2.6
1	A	52	GLU	2.6
1	A	83	HIS	2.6
1	A	149	LYS	2.6
1	B	219	LEU	2.6
1	A	22	TYR	2.6
1	B	120	ASP	2.6
1	A	193	THR	2.6
1	B	251	TYR	2.5
1	A	139	TYR	2.5
1	B	238	SER	2.5
1	B	253	VAL	2.5
1	B	151	ILE	2.5
1	B	23	THR	2.5
1	A	69	LYS	2.5
1	B	147	ASN	2.5
1	B	60	ARG	2.5
1	A	119	LEU	2.4
1	B	203	THR	2.4
1	A	8	ALA	2.4
1	B	218	ALA	2.4
1	B	170	ILE	2.4
1	A	56	ASN	2.4
1	A	185	ASP	2.4
1	B	41	ILE	2.4
1	B	137	LEU	2.4
1	A	15	ASN	2.4
1	B	16	ASN	2.4
1	B	129	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	150	ILE	2.4
1	B	183	ILE	2.4
1	B	49	VAL	2.4
1	B	11	THR	2.3
1	A	116	LYS	2.3
1	A	64	GLN	2.3
1	A	131	SER	2.3
1	B	77	ASN	2.3
1	A	118	LEU	2.3
1	A	258	PHE	2.3
1	B	37	GLU	2.3
1	B	56	ASN	2.3
1	A	230	GLN	2.3
1	A	108	LYS	2.3
1	B	53	ARG	2.3
1	B	192	ILE	2.3
1	B	231	ILE	2.3
1	B	175	SER	2.3
1	B	22	TYR	2.3
1	B	15	ASN	2.3
1	A	37	GLU	2.3
1	A	141	ILE	2.3
1	B	79	ASP	2.3
1	A	134	ILE	2.2
1	A	242	TYR	2.2
1	B	195	ARG	2.2
1	A	191	GLU	2.2
1	B	135	SER	2.2
1	B	209	LEU	2.2
1	B	35	TYR	2.2
1	A	91	ILE	2.2
1	B	200	SER	2.2
1	B	215	SER	2.2
1	B	125	ILE	2.1
1	B	69	LYS	2.1
1	B	82	ARG	2.1
1	A	138	ILE	2.1
1	A	25	LEU	2.1
1	B	118	LEU	2.1
1	A	148	GLU	2.1
1	A	66	LEU	2.1
1	B	9	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	132	ALA	2.1
1	A	247	PHE	2.1
1	B	14	PHE	2.1
1	A	9	LYS	2.1
1	A	33	ASP	2.1
1	A	111	THR	2.1
1	B	158	SER	2.1
1	B	108	LYS	2.1
1	A	60	ARG	2.0
1	A	130	ASN	2.0
1	B	57	ILE	2.0
1	B	226	TYR	2.0
1	A	54	GLY	2.0
1	A	246	ILE	2.0
1	A	29	ASN	2.0
1	B	196	LYS	2.0
1	A	48	LEU	2.0
1	A	137	LEU	2.0
1	A	237	ILE	2.0
1	B	91	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.